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INTRODUCTION TO OPTIMISATION

Office S2.14, Strand Building, Stra

Email: hak-keung.lam@

https://nms.kcl.ac

Nature-Inspired Learning Algorithms (7CCSMBIM)

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1. Aims and Objectives
2. Optimisation
   - Minimisation and Maximisation
   - Local/Global Minimum/Maximum
   - Definition of Optimisation
   - Categories of Optimisation
3. Specific O
   - Least-
   - Linear
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4. Traditional Analytical/Numerical Methods
   - Analytical Optimisation Methods
   - Traditional Numerical Methods
     - Exhaustive Search
     - Nelder-Mead Downhill Simplex Method
     - Gradient Descent
     - Line Minimisation
     - Convergence of Gradient Descent
   - Random-Based Optimisation
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5. Examples

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Aim:

- To review traditional optimisation concept and methods.
- To apply optimisation technique to find the optimal solution to problems.

Objective

- Defi
- To kn

- To appreciate the pros and cons of various traditional op
- To understand the properties of given problems and o problems.

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General Form of (Constrained) Optimisation Problems:

$$\text{Optimise } f(\mathbf{x})$$
$$\text{Subject to (s.t.) } g(\mathbf{x}) \in \Omega \qquad (1)$$

- $f(\mathbf{x})$: cost/objective/fitness function to be optimised (minimised or maximi
  - A
    v
  - It i

  - F
    candidate solution by returning a scalar value. The smaller the scal
    the better the quality of the candidate solution.
- $g(\mathbf{x})$: a set of constraint functions existing in the domain

- $\mathbf{x} = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}$: a vector of decision variables

Optimal Solution:

$\mathbf{x}_{opt} = \arg \min_{\mathbf{x}, g(\mathbf{x}) \in \Omega} f(\mathbf{x})$ (minimisation). $f(\mathbf{x}_{opt}) \leq f(\mathbf{x}) \; \forall \; \mathbf{x} \neq \mathbf{x}_{opt}$

$\mathbf{x}_{opt} = \arg \max_{\mathbf{x}, g(\mathbf{x}) \in \Omega} f(\mathbf{x})$ (maximisation). $f(\mathbf{x}_{opt}) \geq f(\mathbf{x}) \; \forall \; \mathbf{x} \neq \mathbf{x}_{opt}$

$$\min_{\mathbf{x}} f(\mathbf{x}) \quad \Leftrightarrow \quad \max_{\mathbf{x}} -f(\mathbf{x}) \tag{2}$$

where $\mathbf{x} \in R^n$

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Finding the Best Solution:

- Optimisation is the process of adjusting the inputs or characteristics of a device, mathematical process, or experiment to find the minimum or maximum output or result.

- Throughout this module, we address the optimisa a *minimisation problem*.

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$$\min_{\mathbf{x}} f(\mathbf{x}) = ||\mathbf{A}\mathbf{x} - \mathbf{B}||_2^2 \qquad (3)$$

where $\mathbf{x}$ n m n m

Analytic

$f(\mathbf{x}) = \mathbf{x}$

A vector $\mathbf{x}$ minimises $f(\mathbf{x})$: $\nabla f(\mathbf{x}) = 2\mathbf{A}^T\mathbf{A}\mathbf{x} -$

$\Rightarrow \mathbf{x} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{B}$

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \vdots \\ \frac{\partial f(\mathbf{x})}{\partial x_n} \end{bmatrix}$$

Special Case: If the columns of $\mathbf{A}$ are orthogonal to each other, then the solution $\mathbf{x}$ can be obtained as below:

$$x_1 \qquad \frac{\mathbf{B}\cdot\mathbf{a}_1}{\mathbf{a}_1\cdot\mathbf{a}_1}$$

$$\overline{\qquad}$$

$$\overline{\quad n \cdot \quad n}$$

where $\cdot$ denotes the dot product operator; $\mathbf{a}_i$ is a i^{th} column of the matrix A.

Remark: The columns of $\mathbf{A}$ being orthogonal to each other meaning $\mathbf{a}_i \cdot \mathbf{a}_j = 0$ for all $i \neq j$.

$$\min_{\mathbf{x}} f(\mathbf{x}) = \mathbf{c}^T\mathbf{x}$$

$$\text{Subject to } \mathbf{a}_i^T\mathbf{x} \quad b_i, i = 1, \quad , q \tag{4}$$

where $\mathbf{x} = \begin{bmatrix} \vdots \\ x_n \end{bmatrix}$ is a decision variable vector, $=$, $=$ and $b_i \in R$;

b_i is called the “boundary”.

Remark: Equality constraints can be used as well.

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Steps in solving Linear Programming Problems

1. **Problem formulation**
   - Define the decision variables
   - Describe the objective/cost/fitness function (in terms of decision variables)
   -
2. **Gra**
   -
   - Find all corner points of the feasible region (corner-point feasible solutions)

Evaluation
   - Evaluate all corner points of the feasible region (c
     with the objective/cost/fitness function

Return the solution
   - Return the corner point that give the optimal solution (minimum or maximum according to the problem)

- **Solution**: any specification of values for the decision variables.
- **Feasible Solution**: a solution for which *all* th
- **Infea** which
- **Feasible Region**: the collection of all feasible solutions.
- **Optimal Solution**: a feasible solution that has the *most favourable value* of the objective function.

- **Constraint boundary**: a line that forms the boundary of the feasible region by the corresponding constraint.
- **Corn** inters
- Point **corner-point solutions**.
- Points A, B, C, D, and E are **corner-point feasible solutions** (**CPF solutions**).
- Points F, G, and H are **corner-point infeasible solutions**.

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- Each corner-point solution lies at the intersection of two constraint boundaries.
  - With n decision variables, each corner-point solution lies at the

- Two C
  other if t

  - E.g. points A and B are adjacent, while A and C are not adjacent.
  - With n decision variables, two CPF solutions are adjacent if they share $n-1$ constraint boundaries.

- Two adjacent CPF solutions are connected by an **edge** of the feasible region.

Point	x_1	x_2	$Z = 3x_1 + 5x_2$
A	0	0	**0** (minimum)
B			
C			
D			
E	4	0	12

Advantages:

- Simple and easy to understand
- Simple problems can be solved by paper and hand
- Co
- Doe
- Can

Disadvantages:

- Does not give a clue for global minimum/maximum
- Does not work well with discrete variables (integer s
- The cost function and constraints must be linear
- The coefficients of the objective/cost/fitness function and constraints must be constants

$$\min_{\mathbf{x}} f(\mathbf{x}) \tag{5}$$

$$\text{Subject to } g_i(\mathbf{x}) \quad 0, i = 1, \quad , q \tag{6}$$

(7)

where $\mathbf{x} = \begin{bmatrix} x_2 \\ \vdots \\ x_n \end{bmatrix}$ is a decision variable vector;

real-valued functions with at least one of them being nonlinear.

Methods for solving the problem: e.g., Calculus, the method of Lagrange multipliers

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- An extremum can be found by setting the first derivative/gradient of a cost function to zero and solving for the variable values.

- If the second derivative/gradient is greater than zero, the extremum is a minimum, and conversely, if the second derivative is less than zero, the extr
- Sea

step

searched for the global minimum.

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Unconstrained Optimisation:

Given a single variable function $f(x)$,

- $f(x')$ is the **minimum** if $\frac{df(x)}{dx}\Big|_{x=x'} = 0$ and $\frac{d^2f(x)}{dx^2}\Big|_{x=x'} > 0$
- $f(x')$ is the **maximum** if $\frac{df(x)}{dx}\ {}_{x=x'} = 0$ and $\frac{d^2f(x)}{2}\ {}_{x=x'} < 0$

Constrai

$$\min_{x,y,z} f($$

Subject to $g(x, y,$ (8)

Lagrange function: $L(x,y,z,\lambda) = f(x,y,z) + \lambda(g(x,y,z) - c)$

- λ: Lagrange multiplier
- **Stationary point:** $\nabla L(x,y,z,\lambda) = 0$

Example 1 (Unconstrained): Find the minimum of:

$f(x,y) = x\sin(4x) + 1.1y\sin(2y)$

First derivative:

$$\frac{\partial f(x,y)}{}$$

Second derivative:

$$\frac{\partial^2 f(x,y)}{\partial x^2} = 8\cos(4x) -$$

$$\frac{\partial^2 f(x,y)}{\partial y^2} = 4.4\cos(2y) - 4.4y\sin(2y)$$

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Example 2 (Constrained): Find the minimum of:

$f(x,y) = x\sin(4x) + 1.1y\sin(2y)$

Subject to: $x + y = 0$

$$\frac{\partial L(x,y,\lambda)}{\partial x} = \sin(4x) + 4x\,\mathrm{co}$$

$$\frac{\partial L(x,y,\lambda)}{\partial y} = 1.1\sin(2y) + 2.$$

$$\frac{\partial L(x,y,\lambda)}{\partial \lambda} = x + y = 0$$

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Advantages:

- Mathematically elegant tools based on calculus.
- Converge quickly to extremum.
- Pro

Disadva

- Doe
- Difficult to find all the extrema.
- Cannot deal with cliffs and boundaries.
- Does not work well with discrete variables.

This approach requires checking an extremely large but finite solution space with the number of of combinations of different variables given by

$$V = \Pi_{i=1}^{N_{var}} Q_i$$

where

V : numb

N_{var} : tot

Q_i : number of different values that variables i

Example

$N_{var} = 2$,

$Q_1 = 3$ for x_1,

$Q_2 = 3$ for x_2,

$V = Q_1 \times Q_2$

$= 3 \times 3 = 9$

Example 3: Find the minimum of $f(x,y) = x\sin(4x) + 1.1y\sin(2y)$

Subject to: $0 \le x \le 10$ and $0 \le y \le 10$

- Global minimum of -18.5547 at $(x,y) = (0.9039, 0.8668)$
- Sampled at intervals of 0.1 requiring a total of 101^2 function evaluations

Advantages:

- Do not get stuck in local minima with fine enough sampling.

- Work for either continuous or discontinuous variables/functions.

Disadva

- Tak

- The g
- Only practical for a small number of variables in a limit

Refinement:

- Search a coarse sampling first, then progressivel promising regions with a finer searching.

Nelder-Mead Method: A simplex method for finding a *local* minimum of a function of several variables.

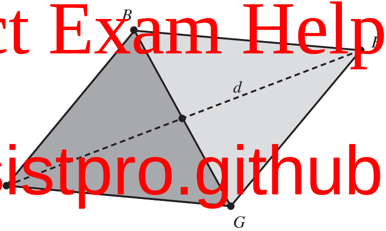
- *Sim* [illegible] and has $N+$ [illegible]
  3-si [illegible]

- *Goa* [illegible]
  1. moving the simplex towards the (local) minimu
  2. surrounding the minimum;
  3. then contracting the simplex around the minimu

  This process will be repeated and stopped until an acceptable error has been reached.

Remark: 4 searching movements: Reflection ; Expansion; Contraction; Shrinking

$$\min_{x,y} f(x,y)$$



Initial Triangle BGW

- Choo
- $\mathbf{B} =$
- $\mathbf{G} =$ $\quad_2 \quad_2$
- $\mathbf{W} = (x_3, y_3)$ (the worst vertex)
- $f(\mathbf{B}) \leq f(\mathbf{G}) \leq f(\mathbf{W})$

Example:

Assume $f(x,y) = x + y$. When $x = 2$ and $y = 3$, $f(2,3) = 2 + 3 = 5$.

Assume $\mathbf{W} = (x_1, y_1) = (4,5)$. $f(\mathbf{W}) = f(4,5) = 4 + 5 = 9$.

So, $f(2,3) < f(\mathbf{W})$ as $5 < 9$.

$$\min_{x,y} f(x,y)$$

Midpoint o

- *Goo*
- $\mathbf{M} = \frac{\quad}{2} \quad \frac{\quad}{2} \quad \frac{\quad}{2}$

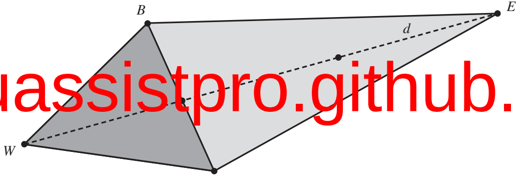
$$\min_{x,y} f(x,y)$$

Reflectio

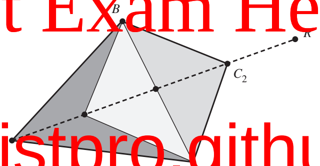
- $\mathbf{R} =$

Expandin

- $\mathbf{E} = \mathbf{R} + (\mathbf{R} - \mathbf{M}) = 2\mathbf{R} - \mathbf{M}$



$$\min_{x,y} f(x,y)$$



Contracti

- Two
- $\mathbf{C}_1$ ... $\frac{\quad}{2}$
- $\mathbf{C}_2 = \frac{\mathbf{M}+\mathbf{R}}{2}$

Shrink towards B

- $\mathbf{S} = \frac{\mathbf{B}+\mathbf{W}}{2}$
- $\mathbf{M} = \frac{\mathbf{B}+\mathbf{G}}{2}$

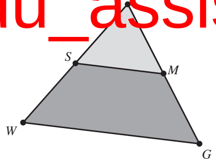


Figure 5: Shrinking.

Traditional Numerical Methods:

Nelder-Mead Downhill Simplex Method

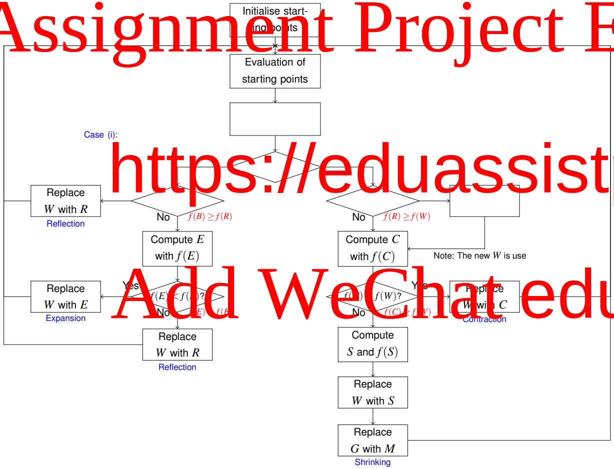


Figure 6: Flowchart of Nelder-Mead Downhill Simplex Method.

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Algorithm 1: Nelder-Mead Downhill Simplex Method (2 dimensional case)

IF $f(R) < f(G)$ THEN Perform `Case (i)` [either reflect or extend];
ELSE Perform `Case (ii)` [either contract or shrink];

begin `Case (i)`
- **if** $f(B$
  - r
- **else**
  - C
  - **if** $f(E) < f(B)$ **then**
    - replace W with E;
  - **else**
    - replace W with R;
  - **end**
- **end**

end

begin `Case (ii)`
- 2;
- or
- **if**
- **el**
  - replace W with S;
  - replace G with M;
- **end**

end

Note: At the end of the process, the B, G and W points need to be updated for the next iteration.

Example 4: Find the minimum of $f(x,y) = x^2 - 4x + y^2 - y - xy$.

Initialization:

- Star
- Eval
  $f(0,$

- $\mathbf{B} = (1.2, 0)$, $\mathbf{G} = (0, 0.8)$ and $\mathbf{W} = (0,$

A better point will be found to replace the verte

Find the Midpoint:

- $\mathbf{M} = \frac{\mathbf{B}+\mathbf{G}}{2} = \frac{(1.2,0)+(0,0.8)}{2} = (0.6, 0.4)$.

Example 4 (cont'd):

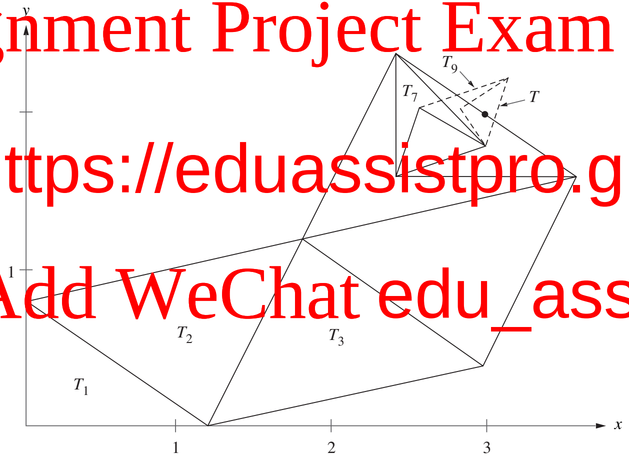
Reflection Point $\mathbf{R} = 2\mathbf{M} - \mathbf{W}$:

- $f(\mathbf{R}$ … se (i))

Expansi

- $f(\mathbf{R}$ … ve in the right direction).
- $\mathbf{E} = 2\mathbf{R} - \mathbf{M} = 2(1.2, 0.8) - (0.6, 0.4)$

Since $f(\mathbf{E}) = f(1.8, 1.2) = -5.88 \leq f(\mathbf{B}) =$
will replace point $\mathbf{W}$. The new triangle has the vertices of $\mathbf{B} = (1.8, 1.2)$, $\mathbf{G} = (1,2,0)$ and $\mathbf{W} = (0, 0.8)$ such that $f(\mathbf{B}) = -5.88$, $f(\mathbf{G}) = -3.36$ and $f(\mathbf{W}) = -0.16$.


y
T_9
T_7
T
1
T_2
T_3
T_1
1
2
3
x

k	Best point	Good point	Worst point
1	$f(1.2, 0.0) = -3.36$	$f(0.0, 0.8) = -0.16$	$f(0.0, 0.0) = 0.00$
2	f		$) = -0.16$
3	f		$) = -3.36$
4	f		$) = -4.44$
5	f		$) = -5.83$
6	f		$) = -6.24$
7	$f(3.0, 1.8) = -6.96$	$f(2.4, 1.6) = -6.72$	$f(2.4, 2.4)$ 6.24
8	$f(3.0, 1.8) = -6.96$	$f(2.55, 2.05) = -$	6.72
9	$f(3.0, 1.8) = -6.96$	$f(3.15, 2.25) = -$	6.7725
10	$f(3.0, 1.8) = -6.96$	$f(2.8125, 2.0375) = -$	6.9525

Table 1: Values of $f(x, y)$ at various triangles.

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$$\min_{\mathbf{x}} f(\mathbf{x}) \quad (9)$$

where $\mathbf{x} \in \; ^n$

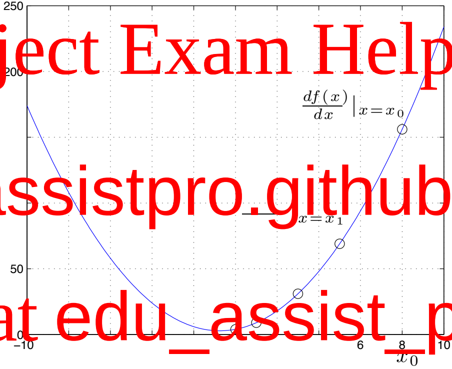
differentia

Update rul

- $\mathbf{x}_{k+1} = \mathbf{x}_k - h_k \;\; f(\mathbf{x})$
- $h_k > 0$ is the *step size*.
- Stopping criteria: $|| \nabla f(\mathbf{x}) || \leq \varepsilon$

and $k < k_{max}$.

$$|| \nabla f(\mathbf{x}) || = \sqrt{\sum_{i=1}^{n} \left(\frac{\partial f(\mathbf{x})}{\partial x_i} \right)^2}$$



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Algorithm: Gradient Descent

input: $f(\mathbf{x}) : \Re^n \to \Re$ a differential function

$\mathbf{x}_0$: an initial solution

output: $\mathbf{x}^*$, a local minimum of the cost function $f(\mathbf{x})$

$k+1$ k k

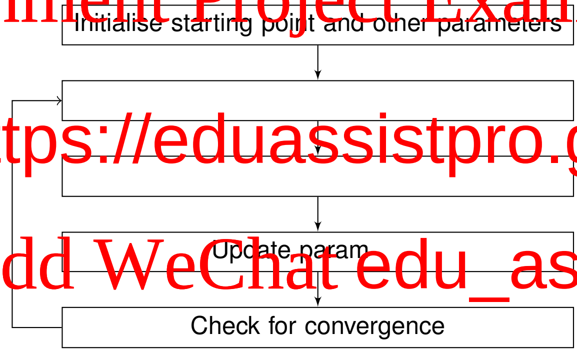
$k \leftarrow k+1$;

end

return $\mathbf{x}_k$;

Table 2: Pseudo Code of Gradient Descent Algorithm.

- An algorithm begins at some random point, and then choose a direction to move until the cost function begins to increase.



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Single Variable Case:

$$\min_x f(x)$$

where $x \in \Re$ and $f(x)$ is a continuously differentiable function.

Taylor Series Expansion at point x_k:

where $f'(x_k) = \frac{df(x)}{dx}\big|_{x=x_k}$ and $f''(x_k) = \frac{d^2 f(x)}{dx^2}$

$f(x) \approx f(x_k) + f'(x_k)(x - x_k) + \frac{1}{2} f''(x_k)(x - x$

$\frac{df(x)}{dx} \approx f'(x_k) + f''(x_k)(x - x_k) = 0$

Update rule:

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$$

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Multiple Variable Case:

$$\min_{\mathbf{x}} f(\mathbf{x})$$

where $\mathbf{x} \in \Re^n$ and $f(\mathbf{x})$ is a continuously differentiable function.

Taylor Se

$f \quad - \quad h.o.t$

where

$\mathbf{x} = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}$ is a point near $\mathbf{x}_k$

$\nabla f(\mathbf{x}_k) = \frac{df(\mathbf{x})}{d\mathbf{x}} \Big|_{\mathbf{x}=\mathbf{x}_k} = \begin{bmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} & \cdots & \frac{\partial f(\mathbf{x})}{\partial x_n} \end{bmatrix}_{\big|\mathbf{x}=\mathbf{x}_k}$

Hessian matrix: $\mathbf{H} = \nabla^2 f(\mathbf{x}) \big|_{\mathbf{x}=\mathbf{x}_k}$ (with elements given by $h_{ij} = \frac{\partial^2 f(\mathbf{x})}{\partial x_i \partial x_j}$)

$f(\mathbf{x}) \approx f(\mathbf{x}_k) + \nabla f(\mathbf{x}_k)(\mathbf{x} - \mathbf{x}_k)^T + \frac{1}{2}(\mathbf{x} - \mathbf{x}_k)\mathbf{H}(\mathbf{x} - \mathbf{x}_k)^T$
$\nabla f(\mathbf{x}) = \nabla f(\mathbf{x}_k) + (\mathbf{x} - \mathbf{x}_k)\mathbf{H} = \mathbf{0}$

Update rule:

- When

decent algorithm.

Advantages:

- Robust and quick convergence.
- Tra

Disadva

- Wor
- Does not guarantee global minimum.
- Does not work well with discrete variables.

- Sensitive to initial guess.
- Trapped in local minimum.

Will the Gradient Descent algorithm converge to the local minimum?

Consider a special case:

$-$

where 0

Gradient: $\nabla f(\mathbf{x}) = \mathbf{Q}\mathbf{x} - \mathbf{b} = \mathbf{Q}(\mathbf{x} - \mathbf{x}^*)$

Solution: $\nabla f(\mathbf{x}) = \mathbf{0} \Rightarrow \mathbf{Q}\mathbf{x}^* - \mathbf{b} = 0 \Rightarrow \mathbf{x}^* =$

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Update rule: $\mathbf{x}_{k+1} = \mathbf{x}_k - h_k \nabla f(\mathbf{x}_k)$

$$f(\mathbf{x}_k - h_k \nabla f(\mathbf{x}_k)) = \frac{1}{2}(\mathbf{x}_k - h_k \nabla f(\mathbf{x}_k))^T \mathbf{Q}(\mathbf{x}_k - h_k \nabla f(\mathbf{x}_k)) - \mathbf{b}^T(\mathbf{x}_k - h_k \nabla f(\mathbf{x}_k))$$

The optim

$$\frac{\partial f(\mathbf{x}_k \ldots}{\ldots k} \ldots \mathbf{0}$$

$$= -\nabla f(\mathbf{x}_k)^T \mathbf{Q}\mathbf{x}_k + h_k \nabla \ldots {}_k) = \mathbf{0}$$

$$= h_k \nabla f(\mathbf{x}_k)^T \mathbf{Q} \nabla f(\mathbf{x}_k) \ldots$$

$$\boxed{h_k = \frac{\nabla f(\mathbf{x}_k)^T \nabla f(\mathbf{x}_k)}{\nabla f(\mathbf{x}_k)^T \mathbf{Q} \nabla f(\mathbf{x}_k)}}$$

Update rule: $\mathbf{x}_{k+1} = \mathbf{x}_k - \frac{\nabla f(\mathbf{x}_k)^T \nabla f(\mathbf{x}_k)}{\nabla f(\mathbf{x}_k)^T \mathbf{Q} \nabla f(\mathbf{x}_k)} \nabla f(\mathbf{x}_k)$

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Difference: $\| \mathbf{x} - \mathbf{x}^* \|_{\mathbf{Q}}^2 = (\mathbf{x} - \mathbf{x}^*)^T \mathbf{Q} (\mathbf{x} - \mathbf{x}^*) \geq 0 \qquad (\mathbf{Q} = \mathbf{Q}^T > 0)$

$$\frac{1}{2} \| \mathbf{x}_{k+1} - \mathbf{x}^* \|_{\mathbf{Q}}^2 = \frac{1}{2} (\mathbf{x}_{k+1} - \mathbf{x}^*)^T \mathbf{Q} (\mathbf{x}_{k+1} - \mathbf{x}^*)$$

$$+ \frac{1}{2} \mathbf{x}^{*T} \mathbf{Q} \mathbf{x}^*$$

$$= \frac{1}{2} \mathbf{x}_{k+1}^T \mathbf{Q} \mathbf{x}_{k+1} - \mathbf{b}^T \mathbf{x}_{k+1} - \frac{1}{2} \mathbf{x}^{*T} \mathbf{Q} \mathbf{x}^* + \mathbf{b}^T \mathbf{x}^*$$

$$= f(\mathbf{x}_{k+1}) - f(\mathbf{x}^*)$$

Objective: $\mathbf{x}_{k+1} \to \mathbf{x}^*$ as $k \to \infty$ (possible?)

$$\frac{1}{2}||\mathbf{x}_{k+1}-\mathbf{x}^*||^2_{\mathbf{Q}} = \frac{1}{2}(\mathbf{x}_{k+1}-\mathbf{x}^*)^T\mathbf{Q}(\mathbf{x}_{k+1}-\mathbf{x}^*)$$

$$= (\mathbf{x}_k - h_k^*\nabla f(\mathbf{x}_k) - \mathbf{x}^*)^T\mathbf{Q}(\mathbf{x}_k - h_k^*\nabla f(\mathbf{x}_k) - \mathbf{x}^*)$$

$$\ldots_k - \mathbf{x}^*)$$

$$\ldots h_k^*\nabla f(\mathbf{x}_k)$$

where $h_k^* = \frac{\nabla f(\mathbf{x}_k)^T\nabla f(\mathbf{x}_k)}{\nabla f(\mathbf{x}_k)^T\mathbf{Q}\nabla f(\mathbf{x}_k)}$ (a scalar, $h_k^* = h_k^{*T}$)

- $(\mathbf{x}_k-\mathbf{x}^*)^T\mathbf{Q}(\mathbf{x}_k-\mathbf{x}^*) = ||\mathbf{x}_k-\mathbf{x}^*||^2_{\mathbf{Q}} = (\mathbf{x}_k-\mathbf{x}^*)^T\mathbf{Q}\mathbf{Q}^{-1}\mathbf{Q}$
- $(h_k^*\nabla f(\mathbf{x}_k))^T\mathbf{Q}(\mathbf{x}_k-\mathbf{x}^*) = (\mathbf{x}_k-\mathbf{x}^*)^T\mathbf{Q}h_k^*\nabla f(\mathbf{x}_k)$
- $(\mathbf{x}_k-\mathbf{x}^*)^T\mathbf{Q}h_k^*\nabla f(\mathbf{x}_k) = h_k^*\frac{\nabla f(\mathbf{x}_k)^T\nabla f(\mathbf{x}_k)}{||\mathbf{x}_k-\mathbf{x}^*||^2_{\mathbf{Q}}}||\mathbf{x}_k-\mathbf{x}^*||^2_{\mathbf{Q}}$
- $h_k^*\nabla f(\mathbf{x}_k)^T\mathbf{Q}h_k^*\nabla f(\mathbf{x}_k) = h_k^{*2}\frac{\nabla f(\mathbf{x}_k)^T\mathbf{Q}\nabla f(\mathbf{x}_k)}{||\mathbf{x}_k-\mathbf{x}^*||^2_{\mathbf{Q}}}||\mathbf{x}_k-\mathbf{x}^*||^2_{\mathbf{Q}}$

$$\|\, \mathbf{x}_{k+1} - \mathbf{x}^* \,\|_{\mathbf{Q}}^2 = \left\{ 1 - \frac{(\nabla f(\mathbf{x}_k)^T \nabla f(\mathbf{x}_k))^2}{\nabla f(\mathbf{x}_k)^T \mathbf{Q} \nabla f(\mathbf{x}_k) \nabla f(\mathbf{x}_k)^T \mathbf{Q}^{-1} \nabla f(\mathbf{x}_k)} \right\} \|\, \mathbf{x}_k - \mathbf{x}^* \,\|_{\mathbf{Q}}^2$$

Converg

$\|\, \mathbf{x}_{k+1}$ [illegible] $i=0$ [illegible] $(\ \ i)$ $(\ \ i)$ $(\ \ i)$ $-$ $(\ \ i)$ $\|\, \mathbf{x}_0 - \mathbf{x}^* \,\|_{\mathbf{Q}}^2$

$$\|\, \mathbf{x}_{k+1} - \mathbf{x}^* \,\|_{\mathbf{Q}}^2 \to 0 \text{ as } k \to \infty?$$

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$$\min_{\mathbf{x}} f(\mathbf{x})$$

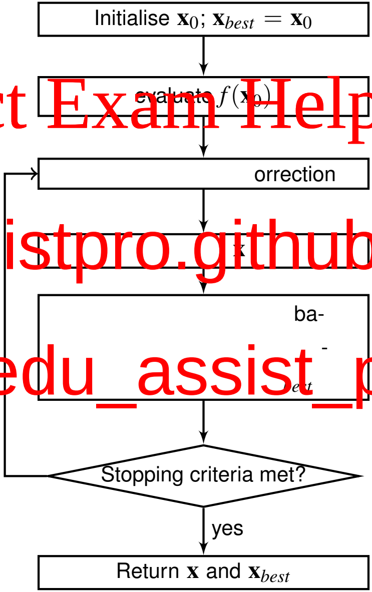
where $\mathbf{x} \in \Re^n$ and $f(\mathbf{x})$ is the cost function.

Must $f(\mathbf{x})$

function?

Property:

- Random elements.



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Update rule:

- $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{D}_k \mathbf{h}_k$.
- Random search direction matrix: $\mathbf{D}_k \in \Re^{n \times n}$ (diagonal matrix).
- Each element of $\mathbf{D}_k$ is either -1 or 1.
- Step siz

Probabili

- Probability of accepting a bad solution.
- Avoid being trapped in the local minimum.

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Boundary:

- Constraint on solution space.
- $\mathbf{x}_{min} \leq \mathbf{x} \leq \mathbf{x}_{max}$

Constrai

- Transf
- Regene

Stopping criterion based on k:

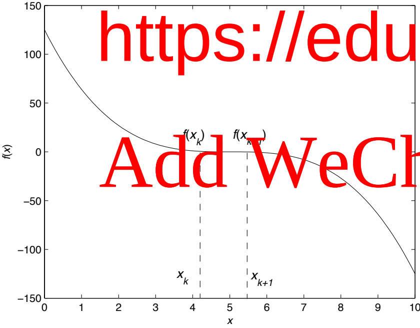
- k_{max} is reached

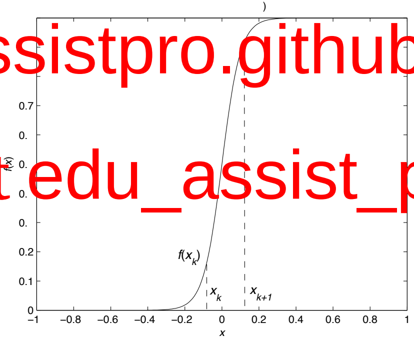
Stopping criterion based on $f(\mathbf{x})$

- $| f(\mathbf{x}_{k+1}) - f(\mathbf{x}_k) | < \varepsilon_f$

Stopping criterion based on $\mathbf{x}$

- $| \mathbf{x}_{k+1} - \mathbf{x}_k | < \varepsilon_x$





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Algorithm: Random Walk Optimisation

input: $f(\mathbf{x}) : \Re^n \rightarrow \Re$; $\mathbf{x}_0$: an initial solution

output: $\mathbf{x}^*$, a local minimum of the cost function $f(\mathbf{x})$

$k \leftarrow 0$; $\mathbf{x}_{best} = \mathbf{x}_0$; *Threshold*;

while STOP-CRIT **and** $k < k_{max}$ **do**

If *rand* < *Threshold* **Then** $\mathbf{x}_{k+1}$ $\mathbf{x}_k$;

Else

If $f(\mathbf{x}_{best}) > f(\mathbf{x}_{k+1})$

End

$k \leftarrow k+1$;

end

return $\mathbf{x}_k$ and $\mathbf{x}_{best}$;

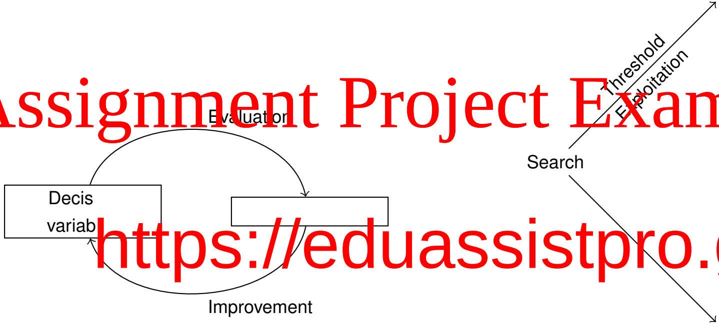
Table 3: Pseudo Code of Random Walk Optimisation.

Example 5: $\min\limits_{\mathbf{x}} f(\mathbf{x}); f(\mathbf{x}) = x_1 \sin(4x_1) + 1.1x_2 \sin(2x_2);$

$\mathbf{x}_0^T = [-1 \quad -1]$; Threshold = 0.9

k	$\mathbf{x}_k^T$	$f(\mathbf{x}_k)$	$\mathbf{x}_{k+1}^T$	$f(\mathbf{x}_{k+1})$	rand()	$\mathbf{x}_{best}$
0	[−1.0000 1.0000]	0.2434	[3.6784 4.4041]	5.8851	0.0739	[−1.0000 −1.0000]
1	[−1.0					−1.0000 −1.0000]
2	[3.60					−1.0000 −1.0000]
3	[3.60					−0.9366 −4.8391]
4	[−0.9					−1.0262 −8.6718]
5	[−1.0262 −8.6718]	−10.3614	[−4.9322 −13.056			62 −8.6718]
6	[−1.0262 −8.6718]	−10.3614	[−2.5688 −8.651			88 −8.6512]
7	[−2.5688 −8.6512]	−11.4441	[−6.9924 −6.592			88 −8.6512]
8	[−2.5688 −8.6512]	−11.4441	[−4.4318 −6.951			88 −8.6512]
9	[−4.4318 −6.9514]	3.4436	[−3.2381 −7.9001]	0.4187	–	[−2.5688 −8.6512]
10	[−3.2381 −7.9001]	0.4187	[−4.9545 −11.2149]	−1.1574	–	[−2.5688 −8.6512]

Traditional Numerical Methods: Random Walk



- lore
  optima.
- **Exploitation:** the ability to concentrate the search around a region to refine a solution.

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Example 6 (function minimisation): $\min_{\mathbf{x}} f(\mathbf{x})$;

$f(\mathbf{x}) = x_1 \sin(4x_1) + 1.1x_2 \sin(2x_2)$; $\mathbf{x}_0^T = [-1 \; -1]$.

Constraints:

- $0 \leq x_1$
- $0 \leq x_2$

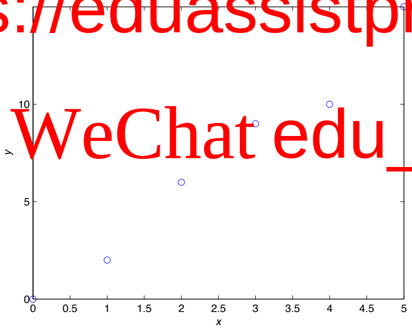
Transformation of Variables

- $y_1 = 5\sin(x_1) + 5$
- $y_2 = 5\sin(x_2) + 5$
- $f(\mathbf{x}) = y_1 \sin(4y_1) + 1.1y_2 \sin(2y_2)$

A constrained optimisation problem becomes an unconstrained optimisation problem

Example 7 (curve fitting): Find the coefficients of an n^{th}-order single-variable polynomial function to best fit the following points (x, y):

x	0	1	2	3	4	5
y	0	2	6	9	10	15



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Example 7 (curve fitting) cont'd:

Any weakness in the random walk optimisation procedure?

What will happen when the number of parameters increases?

Update ru

$\mathbf{x}_{k+1} = \mathbf{x}$

- Allow onl

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Example 7 (curve fitting) cont'd:

- n^{th}-order single-variable polynomial function: $p(x) = \sum_{i=0}^{n} a_n x^n$
- Decision variables: $\mathbf{a} = [a_1, \cdots, a_n]$
- Cost fun N
  - N: nu

- Minimisation problem: $\mathbf{a}$ ( )
- Optimal solution: $\mathbf{a}^* = ?, f(\mathbf{a}^*) \approx 0$

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Example 7 (curve fitting) cont'd:

Control parameters:

Order of polynomial function	3	4	5
No. of decision variables	4	5	6
% of decis			20%

- k_{max} = 1
- $\mathbf{h}_k \leq 0$.
- initial guess of $\mathbf{a}$: all zeros

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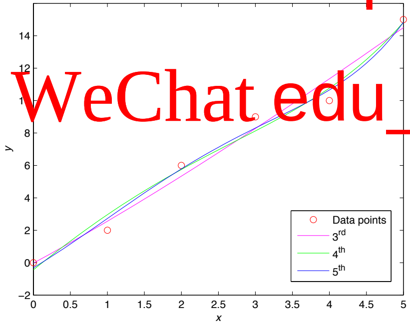
Example 7 (curve fitting) cont'd:

	3^{rd}	4^{th}	5^{th}
$\mathbf{a}^*$	$\begin{bmatrix} 0.00[illegible]6 \\ 0.1134 \\ 2.4785 \\ 0.0256 \end{bmatrix}$	$\begin{bmatrix} 0.[illegible]200 \\ -0.0873 \\ -0.1825 \\ 3.6476 \end{bmatrix}$	$\begin{bmatrix} 0.0058 \\ -0.01[illegible]0 \\ -0.1256 \\ 0.4357 \\ 2.7392 \end{bmatrix}$



Advantages:

- Works with discrete/continuous variables.
- Works with complicated functions.
- Gradient information is not required (can be applied to non-differential functi
- Less s
- Less l algori
- Tends to search for global minimum.

Disadvantages:

- Sensitive to the control parameters.
- Lack of systematic way to choose the control parameters.
- Solution is not repeatable.
- Multiple runs are usually required to verify the solution.
- May not guarantee the convergence.
- Not practical to be implemented online.

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- Understand the concept and procedure of optimisation, i.e., constrained/unconstrained optimisation, minimisation/maximisation problem, local/global solution.
- Get an idea of various optimisation methods, i.e., analytical, numerical, rand
- App
- Able to deal with single/multiple variable optimisation problems.
- Able to define a given problem as optimisation probl objective/cost/fitness function, range of decisio